

Fluctuations in high T_c superconductors with inequivalent conducting layers

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Abstract : The fluctuation contribution to the London penetration depth λ , paraconductivity parallel to the ab -plane (σ'_{ab}) and to the c -axis (σ'_c) and the fluctuation specific heat (C_f) of layered high- T_c superconductors with inequivalent conducting layers are calculated using a Lawrence-Doniach (LD) free energy functional proposed by Bulaevskii and Vagner [1]. Dimensional cross over (DCR) occurs near T_c . The specific temperature dependence of σ'_c differs qualitatively from that of σ'_{ab} . The fluctuation contribution below T_c to the London penetration depth is anisotropic in the ab -plane for YBaCuO compounds

Keywords High temperature superconductors, fluctuations, Lawrence-Doniach model

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1. Introduction

Several experiments point to the importance of fluctuations in the thermodynamics of high temperature superconductors (HTSC). The effect of fluctuations in HTSC's has been observed in magnetization, conductivity, current-voltage and specific heat measurements [2–5] and is quite pronounced owing to the small coherence length $\xi \sim 10 \text{ \AA}$, high transition temperature $T_c \sim 100 \text{ K}$ and layered structure. Since fluctuation effects are more pronounced in lower dimensions it is possible to explore the dimensionality of the fluctuations in the layered superconductors. Paraconductivity data from single crystals of YBaCuO [2,3] exhibit dimensional cross over from 2D to 3D near T_c . Baraduc and Buzdin [6] extended the LD model to the YBaCuO system by introducing two different coupling constants among the CuO_2 layers and has predicted DCR above T_c in paraconductivity measurements. Theodorakis and Tesanovic [7] attributed the positive

curvature of the upper critical field $H_{c2}(T)$ of HTSC's near T_c to the DCR. These authors considered the fact that most of the layered superconductors contain not only superconducting (SC) layers but also non-superconducting (NSC) layers. The Josephson coupling between neighbouring SC and NSC layers makes the order parameter non-zero on the NSC layers as well, through a proximity effect as observed by Briceno and Zettl [8] in Bi 2 : 2 : 1 : 2. Consequently they proposed different order parameters for the inequivalent layers and have shown that the spatial variation of the order parameter from layer to layer in materials whose NSC layers are in proximity of SC layers gives rise to the positive curvature of H_{c2} . Bulaevskii and Vagner [1] also employed a similar model to study the magnetic critical fields and anisotropy of vortex structure in HTSC. In the case of $\text{YBa}_2\text{Cu}_3\text{O}_7$ crystals an elementary cell consists of two types of conducting layers : two isotropic CuO_2 planes (SC) and one layer with CuO chain (NSC). If the coupling of the inequivalent layers is strong enough, effective averaging of the superconducting characteristics of the layers takes place and we obtain the standard model. If on the other hand, the coupling between identical planes is stronger than that between the inequivalent planes we have a model with two weakly coupled order parameters ψ_1 and ψ_2 (see Figure 1). ψ_1 and ψ_2 describe the multiple CuO_2

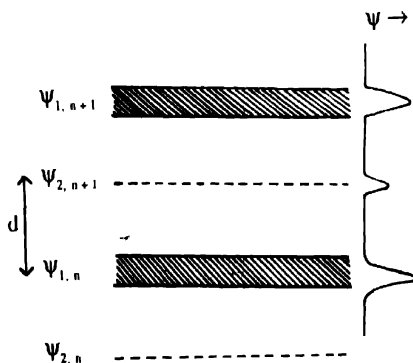


Figure 1. Superconducting and non-superconducting planes in YBaCuO . Shaded area represents CuO_2 double layers and dotted lines the CuO chain layers. The relationship between the order parameter on the SC layer and that on the NSC layer induced by proximity effect is schematically indicated.

layers and metallic layers respectively. The scenario is the same in bismuth and thallium based superconductors also as they contain multiple CuO_2 layers separated by metallic layers (BiO and TlO layers respectively). Like the CuO chain layers in the Yttrium compounds, the BiO and TlO layers in these compounds act as charge reservoirs, dope charges into the CuO_2 layers and enhance the interlayer coupling.

In the present paper, we calculate the fluctuation contribution to the London penetration depth, parallel and perpendicular paraconductivity and fluctuation specific heat based on the LD free energy functional proposed by Bulaevskii and Vagner and study their specific temperature dependence.

2. Fluctuation contribution to the London penetration depth

The free energy expression considered in ref. [1] is

$$\begin{aligned}
 F_s = \sum_n \int & \left[a_1 |\psi_{1,n}^{(\rho)}|^2 + \frac{b_1}{2} |\psi_{1,n}^{(\rho)}|^4 + \frac{\hbar^2}{2m_{\parallel}} \left| \left(\nabla_{\parallel} - \frac{2ie}{\hbar c} A_{\parallel,n} \right) \psi_{1,n}^{(\rho)} \right|^2 \right. \\
 & + a_2 |\psi_{2,n}^{(\rho)}|^2 + \frac{b_2}{2} |\psi_{2,n}^{(\rho)}|^4 + \frac{\hbar^2}{2} \sum_{l=x,y} \frac{1}{m_l'} \left| \left(\frac{\partial}{\partial l} - \frac{2ie}{\hbar c} A_{l,n} \right) \psi_{2,n}^{(\rho)} \right|^2 \\
 & \left. + t \left| \psi_{1,n}^{(\rho)} - \psi_{2,n}^{(\rho)} e^{i\chi_n} \right|^2 + t \left| \psi_{1,n}^{(\rho)} - \psi_{2,n+1}^{(\rho)} e^{-i\chi_n} \right|^2 + \frac{h_n^2}{8\pi} \right] d\rho. \quad (1)
 \end{aligned}$$

$\psi_{i,n}^{(\rho)}$ are the order parameters for layers $i = 1, 2$ in the unit cells numbered by the index n . Subscript 1 refers to the multiple CuO_2 layers and 2 to the metallic layers. $\rho = (x, y)$ and z is the axis perpendicular to the layers. $\chi_n = \frac{2ed}{\hbar c} A_{z,n}$ and $h_n = \text{Curl } A_n$. d is the characteristic distance between the layers.

Let us write

$$a_1 = \alpha_1 (T - T_c) = \alpha_1 \tau T_c$$

and

$$a_2 = \alpha_2 (T - T_c) = \alpha_2 \tau T_c,$$

where $\tau = \frac{(T - T_c)}{T_c}$. For simplicity we assume the same bare critical temperatures for both the inequivalent layers. ∇_{\parallel} is the gradient parallel to the layers. $A_{\parallel,n}$ and $A_{z,n}$ are respectively the components of the vector potential parallel and perpendicular to the n -th layer. t is the coupling coefficient between the neighbouring inequivalent layers. m_{\parallel} is the effective mass of the Cooper pairs in the isotropic CuO_2 planes. The anisotropy of the effective mass due to the chain structure is taken into account in the CuO planes.

We can calculate the fluctuation contribution to the London penetration depth below T_c by writing

$$\begin{aligned}
 \psi_{1,n} &= \frac{|a_1|}{a_1} + \phi_{1,n} \\
 \psi_{2,n} &= \frac{|a_2|}{b_2} + \phi_{2,n}
 \end{aligned}$$

$\frac{|a_i|}{b_i}$ represents the equilibrium value of the order parameter at $T < T_c$ and ϕ_n represents the fluctuation contribution. In the calculation of the fluctuations in high- T_c superconductors for which $\xi(T) \ll \lambda(T)$, we may treat A as constant. This is because the characteristic length scale for changes in A is of the order of $\lambda(T)$ whereas the same for ψ fluctuations is of the

order of $\xi(T)$. After performing Fourier transformation, the fluctuation contribution to the free energy can be written as

$$\delta F_s = \sum_K \left[\frac{a_1}{2} (\phi_{1,K} \phi_{1,-K} + \phi_{1,K}^* \phi_{1,-K}^*) + C_+ |\phi_{1,K}|^2 + \frac{a_2}{2} (\phi_{2,K} \phi_{2,-K} + \phi_{2,K}^* \phi_{2,-K}^*) + D_+ |\phi_{2,K}|^2 \right], \quad (2)$$

where

$$C_{\pm} = a_1 + \frac{\hbar^2}{2m_{\parallel}} \left[q \mp \frac{2e}{\hbar c} A_{\parallel} \right]^2 + 2t \left\{ 1 - \gamma \cos \left[\chi_n \pm \frac{kd}{2} \right] \right\},$$

$$D_{\pm} = a_2 + \frac{\hbar^2}{2m'_x} \left[q \cos \theta \mp \frac{2e}{\hbar c} A_{x,n} \right]^2 + \frac{\hbar^2}{2m'_y} \left[q \sin \theta \mp \frac{2e}{\hbar c} A_{y,n} \right]^2$$

$$+ 2t \left\{ 1 - \frac{1}{\gamma} \cos \left[\chi_n \pm \frac{kd}{2} \right] \right\}$$

and $K = K(q, k)$. q is the inplane wave vector and k is the c -axis wave vector. θ is the angle which the inplane wave vector makes with the x -axis.

We have set $\gamma^2 = \frac{|\phi_{2,K}|^2}{|\phi_{1,K}|^2}$. This introduces an additional phase term which does

not affect the derivation of the final result. The general expression for the fluctuation contribution to the free energy is

$$F_{fl} = -T \ln \int \exp[-\delta H_{eff}(\phi, A)/T] D\phi. \quad (3)$$

Taking δF_s as an effective hamiltonian,

$$F_{fl} = -T \ln \int \exp[(-\delta F_s)(\phi_{1,K}, \phi_{2,K}, A)/T] D\phi_{1,K} D\phi_{2,K}. \quad (4)$$

The additional superconducting current due to fluctuations is

$$j_{fl} = -c \frac{\delta F_{fl}}{\delta A}. \quad (5)$$

Performing the functional integration in (4) over the real and imaginary parts of $\phi_{1,K}$ and $\phi_{2,K}$,

$$F_{fl} = -\frac{T_c}{2} \sum_K \left[\ln \pi^2 T_c^2 (C_+ C_- - a_1^2) + \ln \pi^2 T_c^2 (D_+ D_- - a_2^2) \right]. \quad (6)$$

The London penetration depth is given by the expression

$$\lambda_i^{-2} = -\frac{4\pi j_i}{c A_i}. \quad (7)$$

Since we are interested in finding the linear response, only the vector potential A is considered to be small. Neglecting terms in second and higher powers of A as well as t , changing summation over K in (6) into integration and using eqs. (5) and (7), the fluctuation contribution to the London penetration depth can be calculated as

$$\delta\lambda_l^{-2} = \frac{4e^2 T_c}{\hbar^2 c^2 d} \sum_{j=1,2} \left(\frac{M}{m_l} \right)^{j-1} \left[\ln \left(\frac{2r_j}{3|\tau|} \right) + \gamma^{2i} \left(\frac{1}{4} - \frac{r_j}{2|\tau|} \right) + 2 \frac{(|\tau| + r_j)}{|\tau|} \ln \frac{2(r_j + |\tau|)}{3r_j} \right] \quad (8)$$

$$l = x, y, \quad M = \frac{1}{\pi} \int_0^\pi M_\theta d\theta, \quad M_\theta^{-1} = \left[\frac{\cos^2 \theta}{m'_x} + \frac{\sin^2 \theta}{m'_y} \right],$$

$$i = (-1)^{j-1} \quad \text{and} \quad r_j = \frac{2t}{\alpha_j T_c}.$$

$$\delta\lambda_c^{-2} = \frac{8te^2 dT_c}{\hbar^4 c^2} \sum_{j=1,2} \gamma^j m_j \left[|\tau| + r_j \ln \frac{2|\tau| + r_j}{r_j} \right]. \quad (9)$$

At large τ values ($\tau \gg r$),

$$\delta\lambda_l^{-2} = \frac{4e^2 T_c}{\hbar^2 c^2 d} \sum_{j=1,2} \left(\frac{M}{m_l} \right)^{j-1} \left[\ln \frac{8|\tau|}{27r_j} + \frac{\gamma^{2i}}{4} \right], \quad (10)$$

$$\delta\lambda_c^{-2} = \frac{8te^2 dT_c}{\hbar^4 c^2} \sum_{j=1,2} \gamma^j m_j \left[|\tau| + r_j \ln \frac{2|\tau|}{r_j} \right]. \quad (11)$$

At large τ , specific temperature dependence of $\delta\lambda_l^{-2}$ is different from that of $\delta\lambda_c^{-2}$ because of the presence of an additional term linear in $|\tau|$ in eq. (11).

3. Fluctuation specific heat

If we consider Gaussian fluctuations above T_c , the quartic terms in (1) can be neglected. Setting $A = 0$, the Fourier transform of eq. (1) is performed. The order parameter ψ_2 of the NSC layers arises through a proximity effect. Let us therefore put $\frac{|\psi_{1,K}|^2}{|\psi_{2,K}|^2} = \delta^2$ where

$\psi_{1,K}$ and $\psi_{2,K}$ are the Fourier transformed quantities of $\psi_{1,n}$ and $\psi_{2,n}$ respectively.

$$F_s = \sum_K \left[\varepsilon_1 |\psi_{1,K}|^2 + \varepsilon_2 |\psi_{2,K}|^2 \right] \quad (12)$$

where $\varepsilon_1 = a_1 + \frac{\hbar^2 q^2}{2m_\parallel} + 2t(1 - \delta) - 2t\delta \cos kd$

and $\varepsilon_2 = a_2 + \frac{\hbar^2 q^2}{2M_\theta} + 2t.$

Change in thermodynamic potential

$$\Omega - \Omega_0 = -T \ln \int \exp \left[-\sum_K \left\{ \varepsilon_1 |\psi_{1,K}|^2 + \varepsilon_2 |\psi_{2,K}|^2 \right\} \right] d\psi_{1,K} d\psi_{2,K}. \quad (13)$$

Fluctuation specific heat

$$\begin{aligned} C_f &= -T \frac{\partial^2 (\Omega - \Omega_0)}{\partial \tau^2} \\ &= \frac{T_c}{2} \sum_K \left[\frac{\alpha_1^2}{\varepsilon_1^2} + \frac{\alpha_2^2}{\varepsilon_2^2} \right]. \end{aligned} \quad (14)$$

Changing summation into integration and performing the integration over K ,

$$C_f = \frac{T_c}{2\pi\hbar^2 d} \left[\frac{\alpha_1 m_{\parallel}}{\sqrt{\tau^2 + 4r_1\tau(1-\delta)}} + \frac{\alpha_2 \sqrt{m'_x m'_y}}{\tau + 2r_2} \right]. \quad (15)$$

where $r_1 = \frac{l}{a_1 T_c}$ and $r_2 = \frac{l}{a_2 T_c}$.

The cross over between 3D and 2D regimes is characterised by the parameters r and δ . For $r(1-\delta) \gg \tau$ the specific temperature dependence of C_f becomes 3D.

4. Parallel and perpendicular paraconductivity

The calculation of paraconductivity in this model is straight forward and is done using the time-dependent Ginzburg-Landau (TDGL) equation. Following [6] and [9] parallel fluctuation current can be obtained as

$$j = \frac{\pi \hbar^3 e^2 T_c}{4} \sum_K \left[\frac{\alpha_1}{m_{\parallel}^2} \frac{q(q \cdot E)}{\varepsilon_1^3} + \frac{\alpha_2}{M_{\theta}^2} \frac{q(q \cdot E)}{\varepsilon_2^3} \right]. \quad (16)$$

Performing integration over K , we obtain the fluctuation contribution to the conductivity parallel to the layers

$$\sigma'_{ab} = \frac{e^2}{32\hbar d} \left[\frac{1}{\sqrt{\tau^2 + 4r_1\tau(1-\delta)}} + \frac{2}{(\tau + 2r_2)} \right]. \quad (17)$$

The perpendicular conductivity is calculated using the approach of ref. [10]. Terms in higher powers of l are neglected.

$$\sigma'_c = \frac{e^2 l^2 d}{32\hbar^3} \left[\frac{m_{\parallel}}{(\tau^2 + 4r_1\tau(1-\delta))} + \frac{\sqrt{m'_x m'_y}}{(\tau + 2r_2)^2} \right]. \quad (18)$$

The specific temperature dependence of σ'_{ab} is thus different from that of σ'_c .

5. Discussion

In $\text{YBa}_2\text{Cu}_3\text{O}_7$, the situation of two strongly coupled superconducting CuO_2 layers weakly coupled to the non-superconducting CuO chain layers is realized. The calculations based on the free energy functional (1) describing this situation explain the observation of dimensional cross over in paraconductivity and fluctuation specific heat measurements. There is a clear difference between the temperature dependences of σ'_{ab} and σ'_c . For $\tau \gg r$, the leading term in σ'_{ab} has a τ^{-1} dependence where as σ'_c has a τ^{-2} dependence. The temperature dependence of σ'_c for $\tau \gg r$ is appropriate for a 0D fluctuation regime. The dimensional cross over in the fluctuation regime of C_{fl} and σ'_{ab} takes place exactly at the same temperature as that for σ'_c . However, similar results were also obtained by Baraduc and Buzdin [6] by considering strong coupling between the two CuO_2 planes in the same elementary cell and weak coupling between cells. They have ignored the influence of the chain layers where as the inclusion of the NSC layers is crucial to the calculations in this paper. Qualitatively, both models give the same temperature dependence for fluctuations. However, the magnitude of the cross over temperature and the fluctuation contribution are determined by the inequivalency of the layers combined with weak interlayer coupling. The two models diverge in the determination of the fluctuation contribution below T_c to the London penetration depth and the positive curvature of the upper critical field H_{c2} [12]. The presence of CuO chains in YBaCuO compounds is responsible for the anisotropy of the fluctuations in the ab -plane. In ref. [6] the effect of the chain layers is ignored and as a result the authors obtain isotropic fluctuations in the ab -plane. Therefore, the measurement of fluctuation contribution to the London penetration depth in YBaCuO single crystals will test the validity of the free energy functional (1). The model could be extended to thallium and bismuth based compounds also. Like the CuO chain layers in YBaCuO compounds the double BiO and TlO layers in bismuth and thallium superconductors respectively act as charge reservoirs, dope charge carriers into the CuO_2 layers and enhance the interlayer coupling. However due to the isotropic nature of the BiO and TlO layers, the fluctuations will be isotropic in the ab -plane.

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